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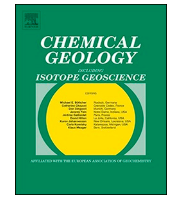

ConwayGEOTRACES

The GEOTRACES Intermediate Data Product 2017☆

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ABSTRACT

The GEOTRACES Intermediate Data Product 2017 (IDP2017) is the second publicly available data product of the international GEOTRACES programme, and contains data measured and quality controlled before the end of 2016. The IDP2017 includes data from the Atlantic, Pacific, Arctic, Southern and Indian oceans, with about twice the data volume of the previous IDP2014. For the first time, the IDP2017 contains data for a large suite of biogeochemical parameters as well as aerosol and rain data characterising atmospheric trace element and isotope (TEI) sources. The TEI data in the IDP2017 are quality controlled by careful assessment of intercalibration results and multi-laboratory data comparisons at crossover stations. The IDP2017 consists of two parts: (1) a compilation of digital data for more than 450 TEIs as well as standard hydrographic parameters, and (2) the *eGEOTRACES Electronic Atlas* providing an on-line atlas that includes more than 590 section plots and 130 animated 3D scenes. The digital data are provided in several formats, including ASCII, Excel spreadsheet, netCDF, and Ocean Data View collection. Users can download the full data packages or make their own custom selections with a new on-line data extraction service. In addition to the actual data values, the IDP2017 also contains data quality flags and 1-σ data error values where available. Quality flags and error values are useful for data filtering and for statistical analysis. Metadata about data originators, analytical methods and original publications related to the data are linked in an easily accessible way. The *eGEOTRACES Electronic Atlas* is the visual representation of the IDP2017 as section plots and rotating 3D scenes. The basin-wide 3D scenes combine data from many cruises and provide quick overviews of large-scale tracer distributions. These 3D scenes provide geographical and bathymetric context that is crucial for the interpretation and assessment of tracer plumes near ocean margins or along ridges. The IDP2017 is the result of a truly international effort involving 326 researchers from 25 countries. This publication provides the critical reference for unpublished data, as well as for studies that make use of a large cross-section of data from the IDP2017.

This article is part of a special issue entitled: "Cycles of trace elements and isotopes in the ocean – GEOTRACES and beyond" - edited by Tim M. Conway, Tristan Horner, Yves Plancherel, and Aridane G. González.

1. Introduction

In 2014, the international GEOTRACES programme (Anderson et al., 2014a, 2014b; SCOR Working Group, 2007; GEOTRACES, 2006; Anderson and Henderson, 2005; Frank et al., 2003; http://www.geotraces.org/) released its first *Intermediate Data Product 2014* (IDP2014, Mawji et al., 2015). The main motivation was to not wait until the end of the programme to issue a final data product. Instead, GEOTRACES wants to create and release a series of intermediate data products at times when the programme is still very active and expanding, both in terms of observational activities as well as the scientific analysis and synthesis of the data produced so far. By releasing and sharing data at early stages, GEOTRACES intends to strengthen and intensify collaboration within the geochemical community itself, but also to attract and invite colleagues from other communities, such as physical, biological and paleo-oceanography, as well as modelling, to apply their unique knowledge and skills to marine biogeochemical research questions.

The release of the IDP2014 was a big success and was widely covered by international news media as well as a broad range of scientific journals (e.g., Morrison, 2014). The data product resulted from a significant effort to combine data from 15 cruises conducted by seven countries. The IDP2014 data cover the Atlantic, Arctic, Southern and Indian oceans and span the 2007 to 2012 period. There are data for 237 hydrographic parameters as well as trace elements and isotopes (TEIs) contributed by 133 scientists from 16 countries. Having such a large group of researchers collaborate on the project and submit high-quality data, sometimes unpublished, was a remarkable achievement.

The IDP2014 is being used widely and has stimulated collaborative research that would not have been possible without such a large, aggregated dataset. Since its release, users worldwide have downloaded the IDP2014 dataset 1410 times. Users of the data product are encouraged to cite the original papers written by the data originators, but the IDP contains significant unpublished data. The publications describing the IDPs thus provide the critical reference for unpublished data, as well as for studies that make use of a large cross-section of data from the IDP. The publication describing the IDP2014 (Mawji et al., 2015) has been cited 43 times, indicating that there is a significant number of scientific studies, such as large-scale modelling and basin-scale to global TEI evaluations, that make use of large portions of the IDP2014 data and could not have been performed otherwise (e.g., Abadie et al., 2017; Chien et al., 2016; Frants et al., 2016; Lerner et al., 2016; Schlitzer, 2016). In particular, the aggregated dissolved iron datasets from IDP2014 facilitated the first rigorous intercomparison of dissolved iron cycling from 13 global ocean models (Tagliabue et al., 2016).

Building on the success of the IDP2014 and following the long-term data product release plan, GEOTRACES released its second intermediate data product (IDP2017) at the Goldschmidt Conference 2017 in Paris. As with the previous product, IDP2017 consists of two parts: (1) the digital data compilation of TEIs as well as standard hydrographic parameters; and (2) the *eGEOTRACES Electronic Atlas* providing section plots and animated 3D scenes of the data. As described in detail below, the IDP2017 contains twice as much data compared to the previous IDP2014. For the first time, the IDP2017 contains significant amounts of biogeochemistry data as well as data for aerosols and rain. All data in the IDP2017 have passed the GEOTRACES standardisation and intercalibration protocols.

2. Intercalibration of data for IDP2017

The direct comparability of GEOTRACES TEI data from any cruise is a prerequisite for assessing global-scale distributions of TEIs, for identifying and quantifying sources and sinks as well as rates of internal cycling, and for providing a baseline against which future changes can be measured. This is also essential for our ability to model natural processes affected by TEIs in the ocean. Therefore, the standardisation and quality control of data sets has always been a cornerstone of the GEOTRACES programme. The importance of intercalibration was illustrated by the U.S. National Science Foundation (NSF)-funded 2003 SAFe iron intercomparison cruise (Johnson et al., 2007), which resulted in widely used consensus material for dissolved trace metals and rare earth elements. Through the GEOTRACES programme, two additional intercalibration cruises were conducted for all the main TEIs and documented in a special issue of *Limnology and Oceanography Methods* in 2012 (Vol. 10 issue 6). Moreover, a cookbook detailing recommended sample collection methods was produced to support intercalibration (http://www.geotraces.org/images/Cookbook.pdf). This document was updated prior to IDP2017 with new intercalibration procedures for TEIs not included in the IDP2014.

While the IDP2014 contained some data that were not quality controlled (identified as tier 2 data), IDP2017 is the first GEOTRACES intermediate data product in which all TEI data have passed the intercalibration procedures and been approved by the Standards and Intercalibration Committee (S&I Committee). This committee is currently a group of eight members approved by the GEOTRACES Scientific Steering Committee. Its members cover a broad range of analytical expertise for the TEIs in IDP2017. In addition, there are element co-ordinators for each group of TEIs who can guide new investigators in developing sample collection and analytical methods (http://www.geotraces.org/sic/s-i-committee/elemental-coordinators).

The intercalibration assessment of the TEI parameters for IDP2017 differed depending on several criteria. For example, the committee had to consider the maturity of the available analytical techniques for a given TEI, the type of TEI in GEOTRACES, the possibly transient nature of the signal, the nature of the data acquisition (e.g., sensor vs. bottle), and the participation in other programmes (such as CLIVAR) that have their own intercalibration procedures.

Irrespective of the quality criteria for individual TEIs, all data were expected to follow certain minimum standards, as shown in Fig. 1. First, written documentation of sampling, measurement and intercalibration procedures was required, provided directly to the S&I Committee as an intercalibration report. This report included details on how samples were collected, how they were processed on board, and how they were stored prior to analyses. This assessment must be carried out for each individual cruise leg, not just for a given laboratory, since the sampling equipment, analytical techniques and analysts may change between cruise legs. The actual assessment was based on the information in these reports and took place during meetings of the S&I Committee.

Second, the methods were assessed for suitability, which included (for example) a check if the procedures were following the cookbook or equivalent, if there were sufficient blank assessments, if detection limits were adequate for the target, and if the laboratory had systems for checking the internal consistency of data, for example replicate analyses, analyses of certified reference materials, or analyses of consensus materials produced from GEOTRACES intercalibration cruises.

Third, the external comparability of the data was assessed. This crucial step comprised an assessment of the crossover stations for key TEIs, that is, those TEIs considered to be of such widespread interest that they should be measured on every GEOTRACES section, and for other TEIs whenever possible. If no crossover stations were possible (e.g., only one cruise had taken place in this region), external comparability had to be demonstrated by participation in a laboratory intercalibration exercise (if such an exercise was available), by the analysis of replicate samples (e.g., where samples were exchanged with another laboratory), and by analyses of certified reference materials or consensus materials. For some TEIs it could also include a comparison to other data in the region of interest. External validation for certain parameters with a core user group outside the GEOTRACES community (e.g., DIC & Alkalinity data, CFCs, sensor data) could also be demonstrated via some other programme (e.g., GO-SHIP, CLIVAR). The assessment of external comparability had to consider the state of the art for any given TEI, with the recognition that the state of the art is changing rapidly, in large part due to GEOTRACES intercalibration activities.

Finally, the S&I Committee assessed jointly if the information provided had demonstrated that the analytical methods reflected the state of the art, and if the data provided had satisfied the quality requirements. If information was missing, the committee contacted the analysts to see if additional information could be provided that would satisfy the need for documentation and quality assurance.

Several parameters have been intercalibrated through new intercalibration exercises (e.g., Si isotopes: Grasse et al., 2017, REE: Behrens et al., 2016; ^{7}Be, particulate TEIs and leachable particulate trace metals; Hg speciation), and new consensus materials have become available for the use of the GEOTRACES community (e.g., Arizona Test Dust for aerosols; Morton et al., 2013). More recently, a sea-ice intercalibration has begun. Results from these on-going intercalibration exercises will be publicised by GEOTRACES as they become available.

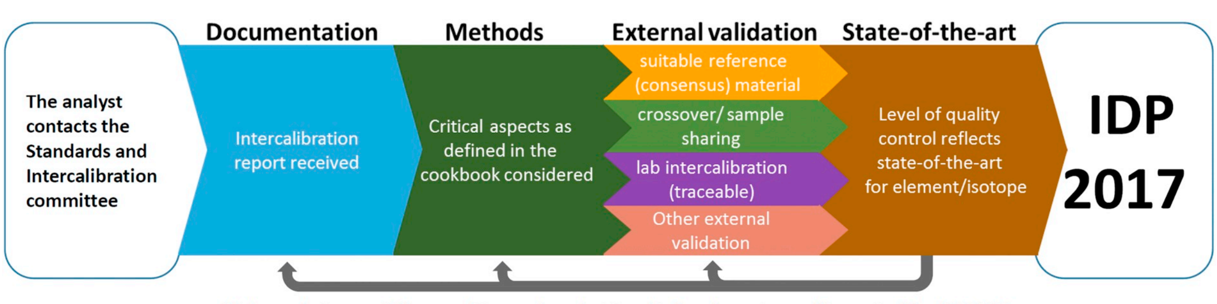

Fig. 1. Flow chart of data assessment for IDP2017.

3. IDP2017 digital data

Creation of the IDP2017 was coordinated and overseen by the GEOTRACES Data Management Committee (DMC). Collation of the cruise data and linkage with extensive metadata was carried out at the GEOTRACES Data Assembly Centre (GDAC) located at the British Oceanographic Data Centre. GDAC received data submissions from four national data centres (Biological & Chemical Oceanography Data Management Office (BCO-DMO; https://www.bco-dmo.org/), Japan Oceanographic Data Centre (JODC; http://www.jodc.go.jp/jodcweb/), LEFE CYBER France (http://www.obs-vlfr.fr/proof/index2.php), NIOZ - Netherlands Data Centre (https://www.nioz.nl/en/research/research-data)) or from GEOTRACES data originators directly. The lead author of this publication carried out the integration of the cruise data into global datasets.

The IDP2017 digital data package consists of three datasets: (1) discrete water sample data; (2) CTD sensor data; and, as a new dataset, (3) aerosol and rain data. The discrete sample and aerosol/rain datasets contain the GEOTRACES TEI data as well as data for a large suite of standard hydrographic data (discrete sample dataset only). The CTD sensor dataset contains high-resolution data from a variety of electronic sensors that are useful for TEI data interpretation and evaluation.

The discrete sample datasets include data from 39 cruises conducted by 11 countries during the 7-year period from 2007 to 2014 (Table 1). Twenty-four of the 39 cruises are new in the IDP2017. The dataset covers the Arctic, Atlantic, Southern, Indian oceans and, the Pacific Ocean (Fig. 2). The best coverage and highest station density is found in the Atlantic, but the new data from the Pacific have already allowed accurate mapping of TEI distributions in parts of the South and North Pacific. In addition to twelve GEOTRACES sections (GA01, GA02, GA03, GA04, GA06, GA10, GA11, GI04, GP02, GP13, GP16, and GP18), which eventually will produce measurements of the large set of GEOTRACES key TEIs (Table 2 in GEOTRACES, 2006), the IDP2017 also includes data from six cruises conducted as part of the International Polar Year (GIPY2, GIPY4, GIPY5, GIPY6, GIPY11, and GIPY13; for an overview of IPY activities see: https://www.icsu.org/publications/understanding-earths-polar-challenges-international-polar-year-2007-2008). For the first time, the IDP2017 also includes GEOTRACES Compliant Data from four cruises (GAc02, GPc01, GPc02, and GPc03) and six GEOTRACES Process Studies (GPpr01, GPpr02, GPpr04, GPpr05, GPpr07, and GPpr10). Typically, these activities produce smaller sets of TEI measurements and sometimes have limited geographical coverage. Nevertheless, compliant data and process studies fill gaps in the overall sampling scheme and provide invaluable data for the quantification of TEI sources and sinks as well as the study of the internal cycling of TEIs. Links to the cruise reports of all cruises in the IDP2017 are provided in Table 2.

In total, the IDP2017 discrete sample dataset contains data for 1810 stations. Of these stations, 817 provide full-depth coverage of the water column. There are data for a total of 458 parameters, including (1) classical hydrographic parameters and tracers such as temperature, salinity, oxygen, nutrients, CFCs, SF_6, Tritium, and He-3, (2) dissolved

Table 1
List of cruises included in the GEOTRACES Intermediate Data Product 2017. Section suffixes denote individual parts of a section. A lower case "c" in the section name (as in GAc01) indicates compliant data while a lower case "pr" (as in GPpr01) indicates a process study. A y in the New column indicates new sections in the IDP2017. Many of the already existing sections had new data added since IDP2014. Cruise locations are illustrated in Fig. 2.

Section	Cruise	Chief scientist	Country	Start date	End date	New
GA01	GEOVIDE	Sarthou, Geraldine	France	15-May-2014	30-Jun-2014	y
GA02 (n)	PE319	Gerringa, Loes	Netherlands	28-Apr-2010	26-May-2010	
GA02 (c)	PE321	Rijkenberg, Micha	Netherlands	11-Jun-2010	08-Jul-2010	
GA02 (s)	JC057	Rijkenberg, Micha	Netherlands	01-Mar-2011	07-Apr-2011	
GA03 (e)	KN199-4	Jenkins, William	USA	15-Oct-2010	04-Nov-2010	
GA03 (w)	KN204-1	Boyle, Edward	USA	06-Nov-2011	11-Dec-2011	
GA04 (n1)	PE370	Rijkenberg, Micha	Netherlands	14-May-2013	05-Jun-2013	y
GA04 (bs)	PE373	Rijkenberg, Micha	Netherlands	13-Jul-2013	25-Jul-2013	y
GA04 (n2)	PE374	Rijkenberg, Micha	Netherlands	25-Jul-2013	11-Aug-2013	y
GA04 (s)	MedSeA	Garcia Orellana, Jordi	Spain	05-May-2013	01-Jun-2013	y
GA06	D361	Achterberg, Eric	UK	07-Feb-2011	19-Mar-2011	y
GA10 (e)	D357	Henderson, Gideon	UK	18-Oct-2010	22-Nov-2010	
GA10 (w)	JC068	Henderson, Gideon	UK	24-Dec-2011	27-Jan-2012	
GA11	M81_1	Frank, Martin	Germany	04-Feb-2010	08-Mar-2010	
GAc01	KN192-5	Saito, Mak	USA	16-Nov-2007	13-Dec-2007	
GAc02	AE1410	Conte, Maureen	USA	31-May-2014	08-Jun-2014	y
GI04	KH09-05	Gamo, Toshitaka	Japan	06-Nov-2009	10-Jan-2010	
GIPY02	AU0703	Griffiths, Brian	Australia	21-Jan-2007	19-Feb-2007	
GIPY04	MD166	Speich, Sabrina	France	08-Feb-2008	24-Mar-2008	
GIPY05	ANT_XXIV_3	Fahrbach, Eberhard	Germany	06-Feb-2008	16-Apr-2008	
GIPY06	AU0806	Rintoul, Steve	Australia	22-Mar-2008	17-Apr-2008	
GIPY11	ARK_XXII_2	Schauer, Ursula	Germany	29-Jul-2007	07-Oct-2007	
GIPY13	ISSS-08	Semiletov, Igor	Sweden	18-Aug-2008	18-Sep-2008	y
GP02	KH12-4	Gamo, Toshitaka	Japan	23-Aug-2012	03-Oct-2012	y
GP13	SS2011-1	Bowie, Andrew	Australia	13-May-2011	05-Jun-2011	y
GP13	TAN1109-2	Boyd, Philip	New Zealand	06-Jun-2011	30-Jun-2011	y
GP16	TN303-EPZT	Moffett, James	USA	25-Oct-2013	20-Dec-2013	y
GP18	KH11-7	Zhang, Jing	Japan	16-Jul-2011	04-Aug-2011	y
GPc01	SO202	Gersonde, Rainer	Germany	07-Jul-2009	29-Aug-2009	y
GPc02	ANT_XXVI_2	Gersonde, Rainer	Germany	27-Nov-2009	27-Jan-2010	y
GPc03	KM1128	Lamborg, Carl	USA	03-Oct-2011	24-Oct-2011	y
GPpr01	TAN0811	Boyd, Philip	New Zealand	15-Sep-2008	04-Oct-2008	y
GPpr02	SS01/10	Hassler, Christel	Australia	23-Jan-2010	15-Feb-2010	y
GPpr04	SO223T	Mohtadi, Mahyar	Germany	09-Sep-2012	08-Oct-2012	y
GPpr05	KM1107	Taylor, Brian	USA	23-Feb-2011	25-Feb-2011	y
GPpr07	LineP_2012-13	Robert, Marie	Canada	14-Aug-2012	30-Aug-2012	y
GPpr07	LineP_2013-18	Robert, Marie	Canada	20-Aug-2013	05-Sep-2013	y
GPpr07	LineP_2014-19	Robert, Marie	Canada	19-Aug-2014	04-Sep-2014	y
GPpr10	TAN1212	Boyd, Philip	New Zealand	23-Sep-2012	23-Sep-2012	y

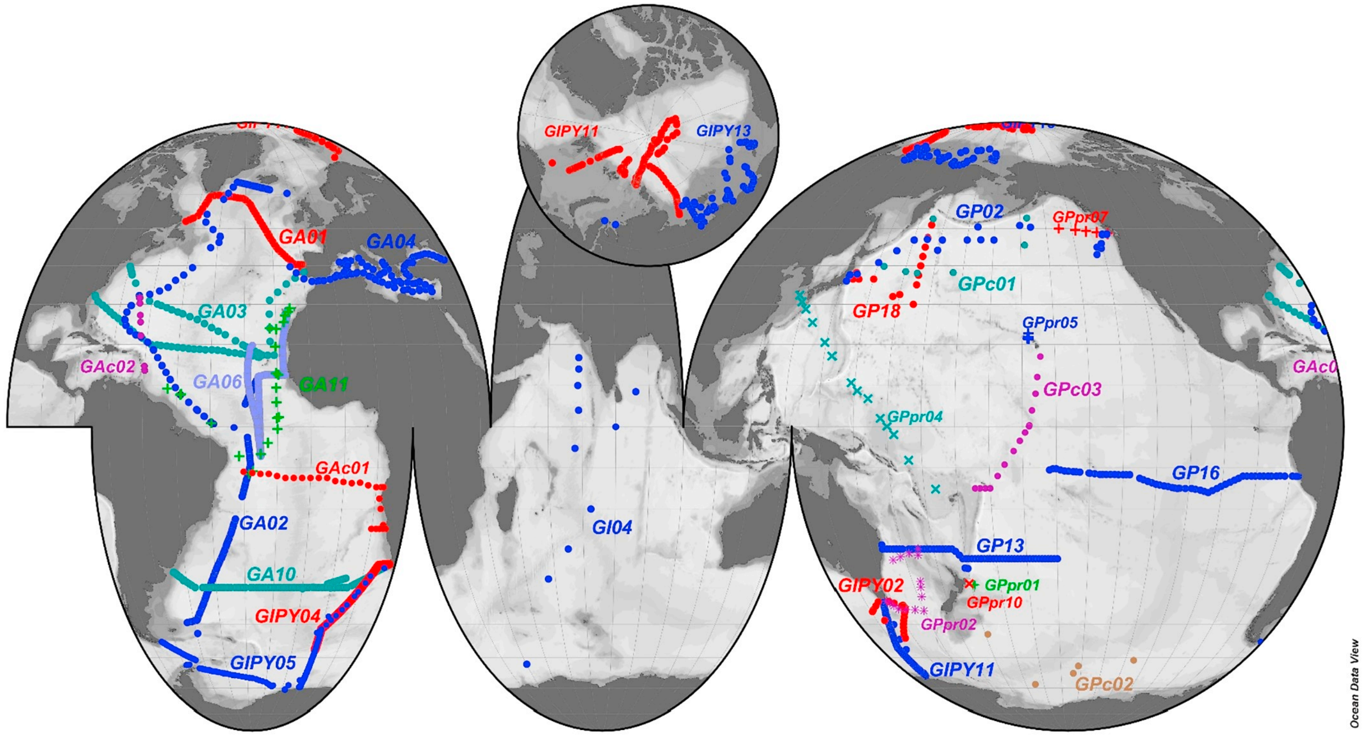

Fig. 2. Map of discrete sample stations included in the GEOTRACES Intermediate Data Product 2017. A lower case "c" in the section name (as in GAc01) indicates compliant data while a lower case "pr" (as in GPpr01) indicates a process study. Different colours and symbols are used to help distinguish between close-by sections. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Table 2
Links to cruise reports of cruises included in the GEOTRACES Intermediate Data Product 2017.

Cruise	Cruise report
AE1410	https://www.bodc.ac.uk/resources/inventories/cruise_inventory/reports/atlanticexplorer_ae1410.pdf
ANT_XXIV_3	https://www.bodc.ac.uk/resources/inventories/cruise_inventory/reports/polarstern_antxxiv3.pdf
ANT_XXVI_2	https://www.bodc.ac.uk/resources/inventories/cruise_inventory/reports/polarstern_ps75.pdf
ARK_XXII_2	https://www.bodc.ac.uk/resources/inventories/cruise_inventory/reports/polarstern_arkxxii2_07.pdf
AU0703	https://www.bodc.ac.uk/resources/inventories/cruise_inventory/reports/auroraaustralis0703.pdf
AU0806	https://www.bodc.ac.uk/resources/inventories/cruise_inventory/reports/auroraaustralis0806.pdf
D357	https://www.bodc.ac.uk/resources/inventories/cruise_inventory/reports/d357.pdf
D361	https://www.bodc.ac.uk/resources/inventories/cruise_inventory/reports/d361.pdf
TN303-EPZT	https://www.bodc.ac.uk/resources/inventories/cruise_inventory/reports/thomasgthompson_tn303.pdf
GEOVIDE	https://www.bodc.ac.uk/resources/inventories/cruise_inventory/reports/pourquoipas_geovide.pdf
ISSS-08	https://www.bodc.ac.uk/resources/inventories/cruise_inventory/reports/isss08.pdf
JC057	https://www.bodc.ac.uk/resources/inventories/cruise_inventory/reports/jc057.pdf
JC068	https://www.bodc.ac.uk/resources/inventories/cruise_inventory/reports/jc068.pdf
KH09-05	https://www.bodc.ac.uk/resources/inventories/cruise_inventory/reports/hakuhomaru_kh-09-5.pdf
KH12-4	https://www.bodc.ac.uk/resources/inventories/cruise_inventory/reports/hakuhomaru_kh12.pdf
KN199-4	https://www.bodc.ac.uk/resources/inventories/cruise_inventory/reports/kn199-4.pdf
KN204-1	https://www.bodc.ac.uk/resources/inventories/cruise_inventory/reports/knorr_kn204_1.pdf
KN192-5	https://www.bodc.ac.uk/resources/inventories/cruise_inventory/reports/kn192-5.pdf
MD166	https://www.bodc.ac.uk/resources/inventories/cruise_inventory/reports/mariondufresne166.pdf
MedSeA	https://www.bodc.ac.uk/resources/inventories/cruise_inventory/reports/angelesalvarino_medsea.pdf
M81_1	https://www.bodc.ac.uk/resources/inventories/cruise_inventory/reports/meteor81_1.pdf
PE319	https://www.bodc.ac.uk/resources/inventories/cruise_inventory/reports/pe319.pdf
PE321	https://www.bodc.ac.uk/resources/inventories/cruise_inventory/reports/pe321.pdf
PE370	https://www.bodc.ac.uk/resources/inventories/cruise_inventory/reports/pelagia_pe370.pdf
PE373	https://www.bodc.ac.uk/resources/inventories/cruise_inventory/reports/pe373.pdf
PE374	https://www.bodc.ac.uk/resources/inventories/cruise_inventory/reports/pe374.pdf
SO202	https://www.bodc.ac.uk/resources/inventories/cruise_inventory/reports/sonne_so202.pdf
SO223T	https://www.bodc.ac.uk/resources/inventories/cruise_inventory/reports/sonne_so223t.pdf
SS01/10	https://www.bodc.ac.uk/resources/inventories/cruise_inventory/reports/southernsurveyor01_2010.pdf
SS2011-1	https://www.bodc.ac.uk/resources/inventories/cruise_inventory/reports/ss2011.pdf
TAN1109-2	https://www.bodc.ac.uk/resources/inventories/cruise_inventory/reports/tangaroa1109.pdf

and particulate trace elements such as Al, Ba, Cd, Cu, Fe, Mn, Mo, Ni, Pb, Zn and Rare Earth Elements (REEs), (3) stable isotopes such as H-2, C-13, N-15, O-18, Si-30, Fe-56, Cd-114, and Nd-143 as well as (4) radioactive isotopes such as Pb-210, Po-210, Th-230, Pa-231, and Th-234. The IDP2017 discrete sample dataset also contains data for a wide range of biogeochemistry parameters, such as HPLC pigments,

Table 3
Number of measurements of selected GEOTRACES parameters in the discrete sample dataset of the IDP2017. Numbers in parentheses indicate the percentage of discrete samples that contain data for that parameter. The "All forms" values include dissolved as well as particulate measurements. For Fe this also includes data for Fe_II and soluble Fe.

Parameter	Number of observations
Trace elements	
Fe	All forms: 12,050 (25.8%); dissolved: 7690 (16.4%)
Mn	All forms: 10,375 (22.2%); dissolved: 6984 (14.9%)
Al	All forms: 10,656 (22.8%); dissolved: 7262 (15.5%)
Zn	All forms: 8787 (18.8%); dissolved: 6932 (14.8%)
Cd	All forms: 10,564 (22.6%); dissolved: 7197 (15.4%)
Pb	All forms: 9181 (19.6%); dissolved: 6157 (13.2%)
Cu	All forms: 7081 (15.1%); dissolved: 3996 (8.5%)
Stable isotopes	
Si-30	All forms: 246 (0.5%); silicate: 246 (0.5%)
O-18	All forms: 1926 (4.1%); water: 1926 (4.1%)
N-15	All forms: 1972 (4.2%); nitrate: 1972 (4.2%)
C-13	All forms: 1113 (2.4%); DIC: 1113 (2.4%)
Radioactive isotopes	
Th-234	All forms: 3768 (8.1%); dissolved plus total particulate: 2520 (5.4%)
Th-230	All forms: 1805 (3.9%); dissolved: 1389 (3.0%)
Pa-231	All forms: 1684 (3.6%); dissolved: 1292 (2.8%)
Pb-210	All forms: 684 (1.5%); dissolved: 493 (0.9%)
Radiogenic isotopes	
Nd-143	All forms: 696 (1.5%); dissolved: 684 (1.5%)

metalloproteomics on filtered particles and metal content of single cells.

A total of 46,794 discrete samples were analysed from the 1810 stations. The average number of depths sampled at each station was 33 but reached up to 182 depths at heavily sampled "super" stations. Table 3 summarises the number of observations for selected parameters, including micronutrients essential to life in the ocean (e.g., Fe, Zn, Cd, Cu), tracers of modern processes in the ocean (e.g., Al, Mn, N-15), tracers significantly perturbed by human activities (e.g., Hg, Pb), and tracers used as proxies to reconstruct the past (e.g., Th-230, Pa-231, Nd isotopes). Data for the micronutrients are most abundant, with the total number of Fe measurements totalling 12,050; of these, 7690 are for dissolved Fe alone. There are 3768 data values for the radioactive isotope Th-234 and around 1800 values for Th-230 and Pa-231.

The CTD sensor dataset contains temperature, salinity, oxygen, fluorescence, transmissometer, turbidity, and photosynthetically active radiation (PAR) data at 1827 stations at 1 m vertical resolution. The fluorescence and transmissometer data provide information on phytoplankton abundance and suspended particle concentrations and are thus important for the interpretation of TEI data. Where calibrated data were not available, raw values are provided. These uncalibrated data are still useful as they reveal the horizontal and vertical extent of phytoplankton patches and suspended particle layers.

For the first time, the IDP2017 contains TEI aerosol and rain data sampled from GEOTRACES cruises. Such data were collected at 243 locations in the Atlantic, Pacific, Mediterranean, and Black Sea (Fig. 3). Data are provided for 99 aerosol parameters, including total TEI concentrations as well as soluble TEI after strong or mild leaching. Also included are size-fractionated TEI concentrations on fine and coarse aerosols. The rain data consist of 68 parameters, including dissolved and total dissolvable TEI concentrations.

In addition to the actual data values, the IDP2017 also contains data quality flags and 1-σ data error values where available. Quality flags and error values are useful for data filtering and statistical data analysis. Quality flags are single character codes reflecting the quality of the respective data value. The IDP2017 uses the IODE quality flag set that is a standard flagging scheme for the exchange of oceanographic and marine meteorological data (www.iode.org/mg54_3). The IODE flagging scheme is generic and simple, only containing the five flags listed in Table 4.

The IDP2017 is an "intermediate" product, and there is clearly a significant amount of further data to come from GEOTRACES cruises,

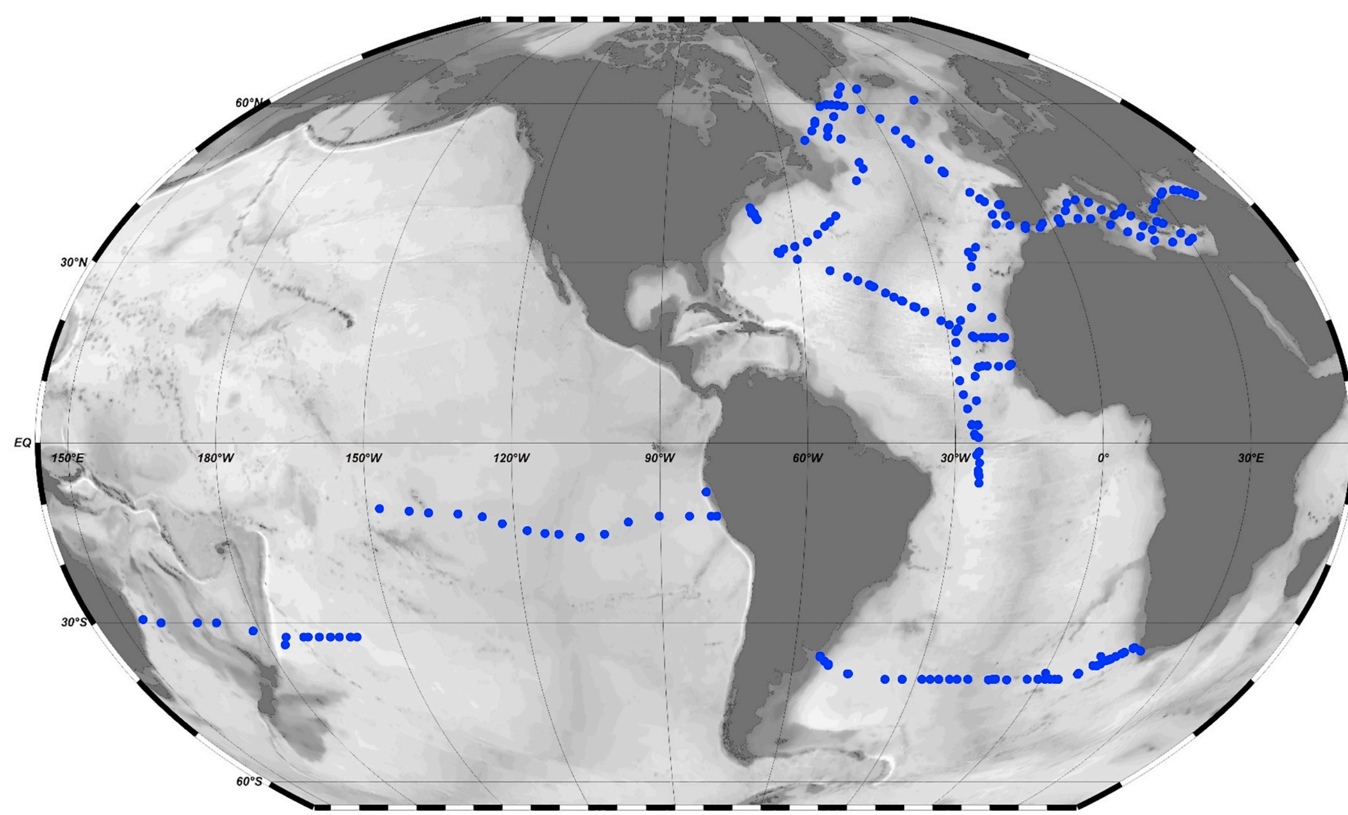

Fig. 3. Map of aerosol and rain stations included in the GEOTRACES Intermediate Data Product 2017.

Table 4
The IODE quality flagging scheme used for the IDP2017.

Value	Flag short name	Definition
1	Good	Passed required QC tests
2	Not evaluated, not available or unknown	Used for data when no QC test performed or the information on quality is not available
3	Questionable/suspect	Failed non-critical metric or subjective test (s)
4	Bad	Failed critical QC test(s) or as assigned by the data provider
9	Missing data	Used as place holder when data are missing

both those represented in the IDP2017, and those sections more recently completed or planned. The IDP2017 contains only those data that were completed and submitted before a cut-off date of December 2016. Further data will be included in subsequent intermediate products (as detailed below) and will significantly augment the data coverage represented in IDP2017.

4. Parameter naming conventions

The overall structure of the databases combined in IDP2017, including a single convention for naming all parameters (variables), was organised by a six-person Parameter Naming Committee (PNC) whose members interacted regularly with the Data Management Committee and with the Standards and Intercalibration Committee. With well over 400 parameters in IDP2017, and with the expectation that the number of parameters could eventually exceed 1000, a structure was sought that would allow users to search intuitively for data, using either tools incorporated into IDP2017 (see "Obtaining IDP2017 Data") or other search engines, utilising a common set of keywords or commands. The structure was designed to accommodate hydrographic and biogeochemical variables as well as TEIs, and to span a range of sampling environments, including seawater, aerosols and rain, while also anticipating the future addition of data from sea ice and sediments. With this in mind, the PNC devised a six-token parameter naming scheme, described in the next two paragraphs, that would encompass all of these characteristics as well as information about operationally defined chemical speciation and physical form of the substance of interest. It is hoped that incorporating all of this information into each parameter name will facilitate searches for highly specific types of data.

The IDP2017 employs the following parameter naming scheme. Standard hydrographic parameters, such as temperature, salinity and oxygen use names as defined in the WOCE/CLIVAR naming convention (CTDTMP, CTDSAL and CTDOXY for temperature, salinity and oxygen

Table 5
Description of the IDP2017 parameter naming scheme.

1	2	3	4	5	6
Element/ compound	[_Oxidation State]	[_Atomic Mass]	_Phase	_DataType	_Sampling System

#	Explanation	Example
1	Element or compound (mandatory)	Fe, Th, DIC, NO3, L1Fe
2	Oxidation state as roman number (optional)	_II, _IV, _III_V_ where III and V are combined
3	Atomic mass (optional); two entries for isotope ratios	_228, _208_204
4	Phase on which element or compound was measured (mandatory); may include two components (e.g., _R_TD_ refers to the Total Dissolvable concentration of a constituent in Rain; _MM_D_ refers to the dissolved concentration of the monomethyl form of a constituent)	_A (aerosol) _C (colloidal) _D (dissolved) _DL (dissolved labile) _F (free (un-complexed)) _LPT (large particulate, total (unleached)) _R (rain) _S (soluble) _SML (soluble mild leach) _SSL (soluble strong leach) _SP (small particulate) _SPL (small particulate, labile fraction) _SPR (small particulate, refractory fraction) _SPT (small particulate, total (unleached)) _T (total) _TD (total dissolvable) _TP (total particulate) _TPL (total particulate, labile fraction) _TPR (total particulate, refractory fraction)
5	DataType (mandatory)	_CONC (concentration) _DELTA (isotope ratio in delta notation) _EPSILON (isotope ratio in epsilon notation) _LogK (log of binding constant of ligand) _RATIO (atomic abundance ratio of isotopes)
6	Sampling system (mandatory)	_BOTTLE (Niskin or similar water sampling bottle) _FISH (trace-metal clean towed surface sampler) _PUMP (either in-situ pump or on-deck pump) _UWAY (ship's underway surface seawater) _HIVOL (high-volume aerosol sampler) _LOWVOL (low-volume aerosol sampler) _FINE_IMPACTOR (size-fractionated aerosols, small fraction) _COARSE_IMPACTOR (size-fractionated aerosols, large fraction) _AUTO (automated aerosol sampler) _MAN (aerosol sampler with manual on-off controls)

from CTD sensors; https://exchange-format.readthedocs.io/en/latest/parameters.html). Other hydrographic parameters use names defined intuitively. Examples are PRESSURE for the CTD pressure at the bottle sample depth, SALINITY, PHOSPHATE, NITRATE, and SILICATE for salinity, phosphate, nitrate and silicate measured on bottle samples. Biogeochemistry parameters in the IDP2017 use names defined by SCOR naming conventions (e.g., HPLC pigments; Roy et al., 2011) or names that intuitively define the parameters (e.g., nifH_UCYN-A_DNA_P_CONC_BOTTLE; concentration of nifH genes from uncultured unicellular cyanobacteria (UCYN-A) particles (P) in a bottle sample).

All other trace elements and isotope names are composed of up to six separate tokens, as follows:

1	2	3	4	5	6
Element/compound	[_Oxidation State]	[_Atomic Mass]	_Phase	_DataType	_Sampling System

Tokens 2 and 3 are optional, while all other tokens are mandatory. The meaning and possible values for all the six tokens are described in Table 5. Example parameter names can be found in Table 6.

The PNC sought to verify that parameter names supplied by contributing investigators complied with the convention described above. In cases where reported data did not comply with a master list of parameters, the PNC would examine the metadata accompanying the original data submission and rename the parameter if appropriate. If there were any question about the correct parameter name, then the PNC would contact the data originator to verify that the parameter had been renamed correctly.

5. Metadata and publication references

The IDP2017 digital datasets include the cruise reports of all the cruises (Table 2). These cruise reports provide detailed documentation of the ship operations, including descriptions of sampling procedures and gear as well as information on the laboratories and principal investigators involved. Access to the cruise reports is very easy. When using the ODV collection version of the IDP2017, a simple mouse click on the *Cruise Report* meta-variable opens the given cruise report and allows viewing in the web browser.

In addition, the IDP2017 also contains, for every parameter and every cruise, a data info file containing information about data originators, sample preparation and analytical methods as well as links to original publications related to the data. These info files are delivered with all IDP2017 output formats and can be viewed easily in the web browser. Access is particularly easy in ODV, where only one mouse click on the info symbol ⓘ is required to open the respective info file in the web browser and obtain detailed information about the data originator and the analytical methods for the clicked parameter and cruise. One more mouse click shows the references of the original publications associated with the given parameter and cruise. Fig. 4 shows an example publication list for parameter Fe_D_CONC_BOTTLE along GP16. Proper linkage of the originator and publication information with the actual data is an important feature of the IDP2017 that makes it easy for users to identify, contact, and acknowledge originators.

The publication links in the IDP2017 info files refer to the reference database of original publications maintained at the GEOTRACES International Programme Office (IPO). This reference database is dynamic and updated whenever new papers are published. Clicking on a reference link in the IDP2017 will always show the up-to-date publication list at the time of the click. Future requests of the publication list related to, for instance, Fe_D_CONC_BOTTLE along GP16 will, in addition to what is shown in Fig. 4, also include new papers published since the Fig. 4 creation date of December 2017. This dynamic inclusion of papers published after the release of the data product was a required feature for the IDP2017, because many datasets were unpublished at the time of data submission.

As a novelty for the IDP2017, the GEOTRACES IPO has made the publication database into a searchable on-line database available on the following GEOTRACES web page: http://www.geotraces.org/library-88/scientific-publications/peer-reviewed-papers. This database is not limited to the IDP2017 as it also includes other publications that are relevant for GEOTRACES research along with Master and PhD dissertations. Three types of search functionalities are available:

(1) Simple search: users can search publications by “author”, “title” or “journal” entering the desired term into a search box,
(2) Advanced search: by means of dropdown menus, users can select publications by “author”, “title”, “GEOTRACES cruise”, “year” or “type of document”, and.

Table 6
Example IDP2017 parameter names.

Parameter name	Parameter description
Fe_D_CONC_BOTTLE	Concentration of dissolved Fe
Fe_II_D_CONC_BOTTLE	Concentration of dissolved Fe(II)
Fe_II_TP_CONC_BOTTLE	Concentration of total particulate Fe(II) determined by filtration from a water sampling bottle
Fe_TPL_CONC_BOTTLE	Concentration of labile particulate iron determined by filtration from a water sampling bottle
Nd_143_144_D_RATIO_BOTTLE	Atom ratio of given isotopes for dissolved Nd
Nd_143_144_D_EPSILON_BOTTLE	Atom ratio of dissolved Nd isotopes expressed in conventional EPSILON notation
Cd_114_110_D_DELTA_BOTTLE	Atom ratio of dissolved Cd isotopes expressed in conventional DELTA notation
Cu_Cu’_D_CONC_BOTTLE	Concentration of dissolved inorganic Cu
Pb_206_204_D_RATIO_BOTTLE	Atom ratio of given isotopes for dissolved Pb
DIC_13_12_D_DELTA_BOTTLE	Atom ratio of given isotopes for dissolved C as DIC in delta notation
DIC_14_12_D_DELTA_BOTTLE	Atom ratio of radiocarbon as dissolved C in DIC in DELTA notation
NITRATE_15_14_D_DELTA_BOTTLE	Atom ratio of given isotopes for dissolved N as nitrate in delta notation
L1_Fe_D_CONC_BOTTLE	Concentration of dissolved L1 Fe-binding ligand
L1_Fe_D_LogK_BOTTLE	Log of the stability constant of L1 Fe
HOMOCYS_D_CONC_BOTTLE	Concentration of dissolved homocysteine
Chl a_HPLC_P_CONC_BOTTLE	Concentration of particulate Chlorophyll a measured using HPLC method
nifH_UCYN-A_DNA_P_CONC_BOTTLE	Abundance nifH Uncultured unicellular cyanobacteria (UCYN-A)

GEOTRACES References

Cruise: GP16
Parameter: Fe_D_CONC_BOTTLE

6 publications found. Export

2017

Fitzsimmons, J. N., John, S. G., Marsay, C. M., Hoffman, C. L., Nicholas, S. L., Toner, B. M., German, C. R., & Sherrell, R. M. (2017). Iron persistence in a distal hydrothermal plume supported by dissolved–particulate exchange. *Nature Geoscience*, *10*(3), 195–201. doi:10.1038/ngeo2900

Heller, M. I., Lam, P. J., Moffett, J. W., Till, C. P., Lee, J.-M., Toner, B. M., & Marcus, M. A. (2017). Accumulation of Fe oxyhydroxides in the Peruvian oxygen deficient zone implies non-oxygen dependent Fe oxidation. *Geochimica et Cosmochimica Acta*, *211*, 174–193. doi:10.1016/j.gca.2017.05.019

John, S. G., Helgoe, J., Townsend, E., Weber, T., DeVries, T., Tagliabue, A., Moore, K., Lam, P., Marsay, C. M., & Till, C. (2017). Biogeochemical cycling of Fe and Fe stable isotopes in the Eastern Tropical South Pacific. *Marine Chemistry*. doi:10.1016/j.marchem.2017.06.003

Sanial, V., Kipp, L. E., Henderson, P. B., van Beek, P., Reyss, J.-L., Hammond, D. E., Hawco, N. J., Saito, M. A., Resing, J. A., Sedwick, P., Moore, W. S., & Charette, M. A. (2017). Radium-228 as a tracer of dissolved trace element inputs from the Peruvian continental margin. *Marine Chemistry*. doi:10.1016/j.marchem.2017.05.008

2016

Boiteau, R. M., Mende, D. R., Hawco, N. J., McIlvin, M. R., Fitzsimmons, J. N., Saito, M. A., Sedwick, P. N., DeLong, E. F., & Repeta, D. J. (2016). Siderophore-based microbial adaptations to iron scarcity across the eastern Pacific Ocean. *Proceedings of the National Academy of Sciences of the United States of America*, *113*(50), 14237–14242. doi:10.1073/pnas.1608594113

2015

Resing, J. A., Sedwick, P. N., German, C. R., Jenkins, W. J., Moffett, J. W., Sohst, B. M., & Tagliabue, A. (2015). Basin-scale transport of hydrothermal dissolved metals across the South Pacific Ocean. *Nature*, *523*(7559), 200–203. doi:10.1038/nature14577

Fig. 4. Example list of publications for parameter Fe_D_CONC_BOTTLE along GP16 as of December 2017.

(3) Parameter search: allows users to access a list of publications by specific TEI. In addition users can also retrieve publications by group of parameters (e.g., Aerosols, Dissolved TEIs, etc.) or by pre-defined subgroups (e.g., dissolved trace elements, etc.).

In each case, search queries for "parameter" or "GEOTRACES cruise" will only list those publications linked to data included in the IDP2017.

6. Obtaining IDP2017 data

The IDP2017 digital data are available in two forms: (1) as full package downloads, or, (2) as customised data subsets using a new online data extraction service. Both methods require users to register (or login if already registered) and agree to IDP2017 usage rules before being able to access and download IDP2017 digital data. The usage rules ask for proper citation of the relevant original papers associated with the particular data used, as well as citation of the IDP2017 data product itself (this paper). Users are also asked to describe the purpose of the IDP2017 data download.

Full packages of the three IDP2017 datasets are available for download at https://www.bodc.ac.uk/geotraces/data/idp2017/. The data are provided in four formats: (1) ASCII text files suitable for usage in standard software, (2) Excel spreadsheet files for Microsoft Excel or similar software, (3) netCDF files suitable for access by models and netCDF readers, and (4) as ODV collections for use with the popular *Ocean Data View* software (https://odv.awi.de).

Users who only need data for a smaller subset of parameters and/or smaller geographical domain can use the new data subsetting and extraction service provided at https://webodv.awi.de/geotraces. After registration and login the user is guided through a three-step procedure. Step 1 allows for subsetting the set of stations to be downloaded by selecting one or more entries from the cruise list, zooming into a specific map domain and/or specifying one or more required parameters (variables). Only stations containing data for all the selected required parameters are included in the output dataset. Step 2 lets users customise the set of parameters (variables) to be included in the download file. This is done using a hierarchical tree of parameter groups and individual parameters. Users open/close parameter groups by clicking the +/− symbols. All parameters of a given group are selected/unselected by clicking the specific group box; individual parameters are selected/unselected by clicking the box of the individual parameter. A *Selection status* box always shows the currently selected numbers of stations and parameters (variables) to be included in the download file. Step 3 lets users choose among four data output formats (ASCII, ODV collection, netCDF, or WOCE WHP exchange) and initiate the actual data download. Selection settings are remembered when a user exits the session and are restored when logging in again later.

7. eGEOTRACES electronic atlas

The *eGEOTRACES Electronic Atlas* is the visual component of the IDP2017 and provides 593 section plots (Fig. 5) and 132 animated 3D scenes (Fig. 6) for many (but not all) of the parameters in the IDP2017. All plots are based on the digital data in the IDP2017, but data values flagged as *Questionable/suspect* or *Bad* (see Table 4) were filtered out and not used for the plots. The *eGEOTRACES* website http://egeotraces.org/ provides a dynamic map, where users start by selecting a data group and a tracer of interest. Sections containing a plot for the selected tracer are highlighted in red in the map, and basins containing a 3D animation for the selected tracer are highlighted in blue. Clicking on a red section label or a blue basin label will show the respective section plot or play the respective 3D scene. All section plots and 3D scenes show the names of scientists who produced or are responsible for the data. This makes it easy for users to identify and acknowledge data producers.

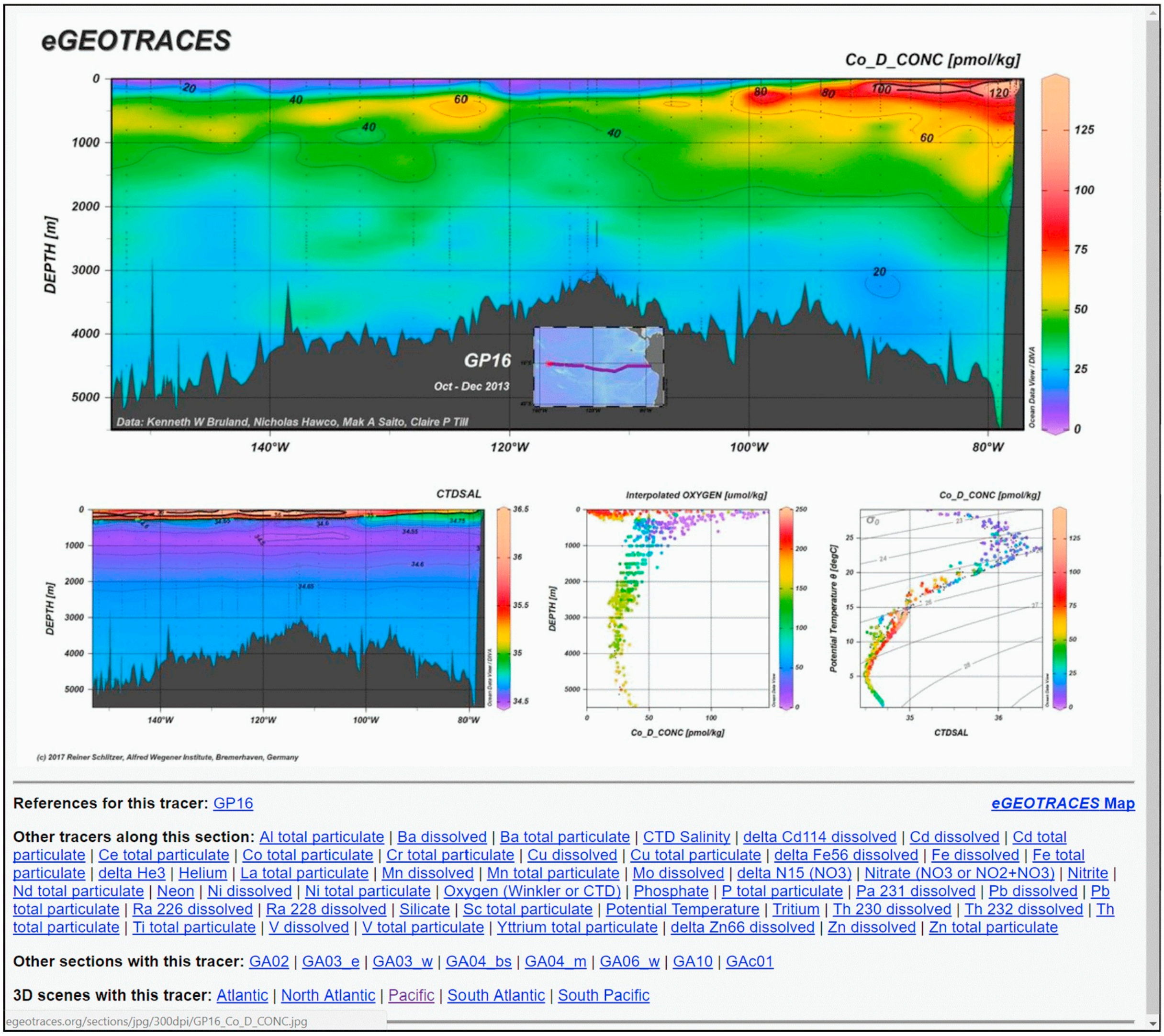

Fig. 5. Example eGEOTRACES section page.

Further clicking on a section plot loads a high-resolution version of the image, which can be saved for use in publications and presentations. The browser's *Back* button is used to return to the original section page. When viewing a rotating 3D scene clicking the *Larger-size Video* link produces a blown-up version of the animation. Clicking the *Normal-size Video* link at the bottom of the blown-up animation returns to the original size. An options bar appears when the mouse is over the 3D animation. Elements on the options bar can be used to stop the animation at arbitrary angles and quickly choose other viewing angles. Some browsers also allow download of the 3D movie file.

All section and 3D animation pages contain groups of links near the bottom of the page. These include (a) links to other tracers along this section or in this scene, (b) other 3D scenes with this tracer, and (c) other sections with this tracer. These links greatly facilitate switching between and comparing of different tracers, sections, and 3D scenes. All section plots use the same window layout, and the different section plots perfectly match when switching between tracers. The links under category (c) allow easy transitions between section plots and 3D animations.

Section and 3D scene pages also contain links to the original publications associated with the given tracer and section. Clicking on these links shows the current list of publications from the dynamically updated reference database maintained at the GEOTRACES IPO (see above).

eGEOTRACES provides quick overviews of the distributions of many geochemically relevant tracers. The 3D scenes provide geographical and bathymetric context crucial for correctly assessing the extent and origin of tracer plumes as well as for inferring processes acting on the tracers and shaping their distribution. The numerous links to other tracers, sections, and basins found on section plots and 3D animations allow quick switching between tracers and domains, and facilitate comparisons between tracers. In addition to the benefit for scientific research, *eGEOTRACES* and its visual material can also help in teaching and outreach activities. The *eGEOTRACES* visuals can also help convey societally relevant scientific results to interested non-scientists and policy makers.

Images or 3D movies from the *eGEOTRACES* Atlas can be used free of charge for non-commercial purposes, such as in scientific publications, posters, presentations and teaching activities, as long as the source is cited as follows: *Schlitzer, R., eGEOTRACES - Electronic Atlas of GEOTRACES Sections and Animated 3D Scenes, http://egeotraces.org, 2017*. Users must not remove the names of data producers and graphics creator. High-resolution images of the 3D scenes are available on request.

8. Summary

The new IDP2017 is a significant improvement over the earlier IDP2014 and roughly doubles the number of included cruises, stations, samples and parameters. The IDP2017 is a truly international product containing data from 326 researchers from 25 countries. The IDP2017

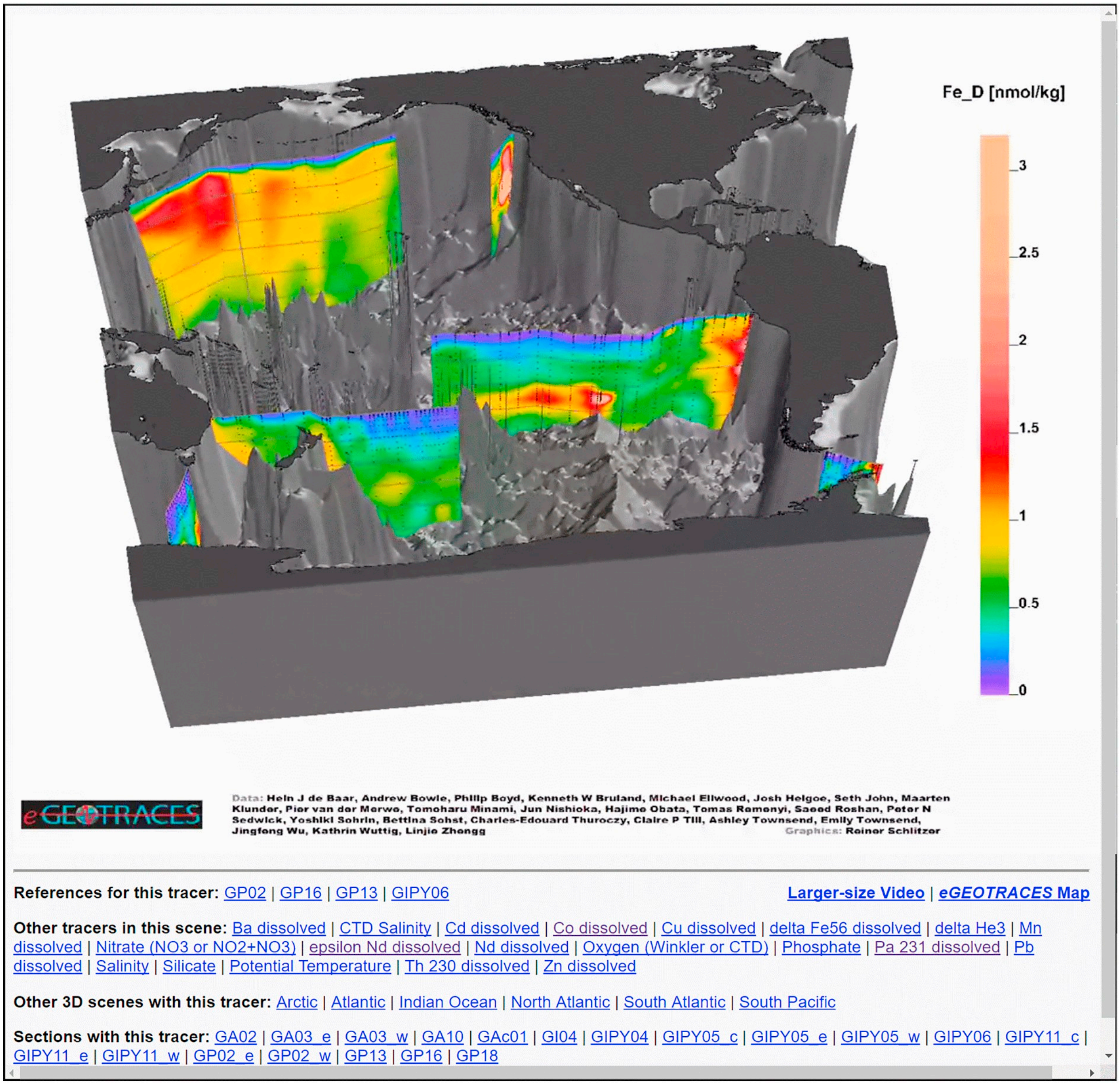

Fig. 6. Example eGEOTRACES 3D scene.

provides data for the Pacific Ocean, and the Mediterranean and Black seas, in addition to Atlantic, Arctic and Indian Oceans that were already represented in the previous data product. For the first time, the IDP2017 contains significant amounts of biogeochemistry data as well as TEI data for aerosols and rain. As before, users can obtain complete IDP2017 data sets as bulk downloads. Alternatively, there is now a customisable online data extraction service that allows data selections by domain, GEOTRACES sections, as well as parameters of interest. The extractor delivers smaller, more manageable data packages.

GEOTRACES invites and promotes use of the IDP2017 in the widest possible sense and envisages intensified collaboration within the marine geochemical community and beyond. Availability of large integrated and quality-controlled datasets, such as the IDP2017, enables a much wider range of studies than would be possible with individual single-cruise data alone.

The new, updated *eGEOTRACES* electronic atlas now contains more than 590 section plots (compared to 330 in IDP2014) and more than 130 animated 3D scenes (95 in IDP2014). Section and 3D scene pages are interlinked, and switching between different GEOTRACES sections, ocean basins and parameters is achieved with simple mouse clicks. *eGEOTRACES* section and 3D scene pages are now connected to the GEOTRACES publication database, easily providing with a simple mouse click up-to-date reference lists to the original publications related to the displayed data. This feature makes identification of data originators easy and encourages proper citation or initiation of collaborative research.

The animated 3D scenes in the *eGEOTRACES Atlas* show large amounts of data in an intuitive way and with geographic and bathymetric context, thereby providing quick large-scale overviews of TEI distributions and helping the scientific interpretation of TEI data. In addition, these animations are also appealing to a wider target community, including scientists from other disciplines or policy makers, as well as interested members of the general public. GEOTRACES encourages wide usage of *eGEOTRACES* visuals for all purposes, including teaching and outreach.

The IDP2017 is the second in a series of planned intermediate data products, with the next scheduled for release in 2021. Future data products will extend the geographical coverage by including data from new GEOTRACES cruises, as well as providing additional data from existing cruises for parameters that take longer to measure and complete. GEOTRACES invites user feedback (ipo@geotraces.org) on the IDP2017 to help make the next IDP an even more useful product.

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